

Synthesis, Crystal Structure and Theoretical Calculations of a Three-dimensional Supramolecular Cadmium(II) Coordination Polymer

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ABSTRACT A new metal-organic cadmium coordination polymer $[\text{Cd}(\text{pzdc})_{0.5}(\text{L})]_n \cdot n\text{H}_2\text{O}$ (**1**, H_2pzdc = pyrazine-2,3-dicarboxylic acid, HL = 3-(2-pyridyl)pyrazole) has been successfully synthesized under hydrothermal conditions. The structure has been determined by single-crystal X-ray diffraction analysis, elemental analyses, IR and fluorescence spectrum. Brown crystals crystallize in the orthorhombic system, space group $Fdd2$ with $a = 11.2636(9)$, $b = 38.296(3)$, $c = 10.5795(8)$ Å, $V = 4563.5(6)$ Å³, $\text{C}_{11}\text{H}_9\text{CdN}_4\text{O}_3$, $M_r = 357.62$, $D_c = 2.082$ g/cm³, $\mu(\text{MoK}\alpha) = 1.924$ mm⁻¹, $F(000) = 2800$, $Z = 16$, the final $R = 0.0169$ and $wR = 0.0443$ for 2106 observed reflections ($I > 2\sigma(I)$). It shows a two-dimensional network structure and extends into a three-dimensional supramolecular framework through π - π stacking interactions. Moreover, we analyzed Natural Bond Orbital (NBO) by using the PBE0/LANL2DZ method built in Gaussian 03 Program. The calculation results showed obvious covalent interaction between the coordinated atoms and Cd(II) ion.

Keywords: hydrothermal synthesis; crystal structure; Cd(II) complex, natural bond orbital;

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1 INTRODUCTION

The designed synthesis and characterization of metal-organic coordination polymers have gained important progress in supramolecular chemistry and material chemistry^[1~8]. The increasing interest in this field is justified not only for their particular beauty and intriguing structural diversities of architecture, but also for their potential applications as catalytic, conductive, luminescent, magnetic, spin-transition, non-linear optical or porous functional materials^[9~16]. The combination of metal ions with neutral and anionic mixed bridging

ligands makes the assembly process more controllable than a single ligand. The prospect of introducing the second or more organic ligands into a reaction system provides further impetus for researches on metal-organic supramolecular frameworks. The construction of supramolecular architectures through selective and directional non-covalent forces such as hydrogen bonding, $\pi \cdots \pi$ and C–H $\cdots \pi$ interactions in metal-organic frameworks arouses considerable contemporary interest owing to their potential applications as functional materials.

The hydrothermal technique is well suitable to the preparation of crystals of synthetic minerals, new inorganic materials, and organometallic coordination polymers. Of particular interest to us is the construction of transition metal polymers with new structural features by utilizing hydrothermal synthesis. We report here the preparation and crystal structure of the title complex $[\text{Cd}(\text{pzdc})_{0.5}(\text{L})]_n \cdot n\text{H}_2\text{O}$ (**1**), which exhibits a 3D supramolecular network through hydrogen bonds and π - π stacking interactions.

2 EXPERIMENTAL

2.1 Materials and instruments

All chemicals were commercially purchased and used without further purification. Elemental analyses of C, H and N were performed on an Elementar Vario III Elemental Analyzer. IR spectrum was recorded in the range of $4000 \sim 400 \text{ cm}^{-1}$ on a Nicolet 6700 spectrometer using a KBr pellet. Powder X-ray diffraction (PXRD) patterns were collected in the 2θ range of $5 \sim 50^\circ$ with a scan speed of 0.1° s^{-1} on a Bruker D8 Advance instrument using $\text{CuK}\alpha$ radiation ($\lambda = 1.54056 \text{ \AA}$) at room temperature. The fluorescent studies were carried out on a computer-controlled JY Fluoro-Max-3 spectrometer at room temperature.

2.2 Synthesis

A mixture of H_2pzdc (0.067 g, 0.4 mmol), HL (0.030 g, 0.2 mmol), $\text{Cd}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (0.11 g, 0.4 mmol) and 18 mL H_2O was adjusted to $\text{pH} \approx 7$ with 40% NaOH, sealed in a Teflon-lined stainless-steel vessel and heated to 150°C for 5 days, followed by slow cooling (a descent rate of 5°C/h) to room temperature. Brown block crystals were obtained. Yield of 41%. Anal. Calcd. for $\text{C}_{11}\text{H}_9\text{CdN}_4\text{O}_3$: C, 36.94; H, 2.54; N, 15.67%. Found: C, 36.05; H, 2.01; N, 15.07%. IR (cm^{-1}): 3609(w), 3478(w), 2360(w), 1629(s), 1601(m), 1567(w), 1519(w), 1471(w), 1452(m), 1432(w), 1378(w), 1365(w), 1350(w), 1285(w), 1259(w), 1231(w), 1201(w), 1157(w), 1122(m), 1095(w), 1074(w), 1067(w), 1051(w), 1011(w), 978(w), 946(w), 880(w), 851(w), 822(w), 790(w), 752(m), 737(w), 709(w), 694(w), 670(w), 648(w), 638(w), 567(w), 509(w), 473(w), 444(w), 436(w).

2.3 X-ray crystallography

All diffraction data of complex **1** were collected on a Bruker/Siemens Smart Apex II CCD diffractometer with graphite-monochromated MoK α radiation ($\lambda = 0.71073$ Å) at 293(2) K. Data reductions and absorption corrections were performed using the SAINT and SADABS programs, respectively. The structure was solved by direct methods with SHELXS-97 program^[17(a)] and refined by full-matrix least-squares techniques on F^2 with SHELXL-97^[17(b)]. All non-hydrogen atoms were refined anisotropically and the hydrogen atoms of organic ligands were generated geometrically. For **1**, a total of 6024 reflections were collected in the range of $2.13 \leq \theta \leq 26.13^\circ$, of which 2133 were independent ($R_{\text{int}} = 0.0126$). The final $R = 0.0169$ and $wR = 0.0443$ for observed reflections with $I > 2\sigma(I)$, and $R = 0.0172$ and $wR = 0.0444$ for all data with $(\Delta\rho)_{\text{max}} = 0.796$ and $(\Delta\rho)_{\text{min}} = -0.335$ e Å⁻³. Selected bond lengths and bond angles of complex **1** are shown in Table 1.

3 RESULTS AND DISCUSSION

3.1 Structural description

Single-crystal X-ray diffraction analysis displays that compound **1** crystallizes in $Fdd2$ space group and consists of a two-dimensional network structure. There are one Cd(II) ion, one L ligand, half H₂pzdc ligand and one crystal water molecule in the asymmetric unit (Fig. 1). The Cd(1) ion is coordinated by three nitrogen atoms from two different L ligands, one nitrogen atom from pzdc ligand in the equatorial plane (Cd(1)–N(1A) = 2.252(3), Cd(1)–N(2) = 2.268(3), Cd(1)–N(3) = 2.371(2), Cd(1)–N(4) = 2.416(3) Å) and one oxygen atom from the pzdc ligand, one oxygen atom from another pzdc ligand at the axial site (Cd(1)–O(1) = 2.514(2), Cd(1)–O(2B) = 2.273(2) Å). The coordination angles around Cd(II) ion are in the range $67.59(9) \sim 167.33(9)^\circ$.

In the crystal structure of complex **1**, each molecule of L binds two cadmium(II) ions through a bidentate-monodentate mode, utilizing two nitrogen atoms to connect one cadmium(II) ion, utilizing one nitrogen atom to connect another cadmium(II) ion, whereas the H₂pzdc ligands adopt a μ_6 coordination mode, with two carboxylate groups utilizing four oxygen atoms to connect four different cadmium(II) ions, with two nitrogen atoms bridging two different cadmium(II) ions. The coordination mode of the H₂pzdc molecule in **1** is different from that in our previously reported compound $[\text{Zn}(\text{pzdc})(\text{mbix})]_n \cdot n\text{H}_2\text{O}$ ^[18]. As a result, four Cd(II) ions are linked by two pzdc and two L ligands, and each pair of the tetranuclear subunits are bridged by pzdc ligands to yield a two-dimensional network structure, as depicted in Fig. 2. The Cd(1) ion exhibits a distorted octahedral coordination architecture.

Further analysis of the crystal packing revealed π - π interactions in complex **1** between N(3)C(4)C(5)C(6)C(7)C(8) pyridine ring of the L ligand. The centroid-to-centroid distances are 3.931(3), 3.929(3) Å and perpendicular distances are 3.411(2), 3.484(2) Å, and the dihedral angle is 6°. Therefore, through π - π interactions, the two-dimensional networks are further extended into a three-dimensional supramolecular framework (Fig. 3).

3.2 IR analysis of complex 1

IR spectrum of **1** shows a broad absorption band at 3478 cm⁻¹, corresponding to the H \cdots O stretching of crystal water molecule in the complex. The C–N absorption peaks of pyridine can be observed at 1350 cm⁻¹. Asymmetric and symmetric COO⁻ stretching modes of the lattice pzdc²⁻ anion were evidenced by very strong, slightly broadened bands at 1601 and 1452 cm⁻¹[19], which is consistent with the results of X-ray analysis.

3.3 Powder X-ray diffraction (PXRD)

To confirm the phase purity of complex **1**, powder X-ray diffraction (PXRD) patterns were recorded for **1**, and it was comparable to the corresponding simulated patterns calculated from the single-crystal diffraction data (Fig. 4), indicating a pure phase of bulky sample.

3.4 Photoluminescent properties

Luminescence property is very significant in photochemistry and photophysics[20, 21]. So, in this study, we measured the solid-state photoluminescence spectra of **1** (Fig. 5) at room temperature. Excited by 440 nm, complex **1** exhibits blue emission with the maximum peak at 495 nm. In order to study the nature of these emission bands, we first analyzed the photoluminescence properties of free L, H₂pzdc ligands, and confirmed that they do not emit any luminescence in the range of 400~800 nm. Therefore, on the basis of the previous literature[22], the emission band could be vested to the emission of ligand-to-metal charge transfer (LMCT). Owing to its strong fluorescent intensity, **1** seems to be a good candidate for novel hybrid inorganic-organic photoactive materials.

4 THEORETICAL CALCULATIONS

The calculations in this manuscript were conducted with the Gaussian 03 program[23]. The parameters of the molecular structure for calculation were all root in the experimental data of complexes **1** and **2**. Natural bond orbital (NBO) analysis was carried out by density functional theory (DFT)[24] with the PBE0[25-28] hybrid

functional and the LANL2DZ basis set^[29].

The major natural atomic charges, natural electron configuration, Wiberg bond indices and NBO bond orders (a.u) for complex **1** are shown in Table 2. It is shown that the electronic configurations of Cd(1) ion, N and O atoms are $5s^{0.29}4d^{9.98}5p^{0.30}$, $2s^{1.34\sim 1.41}2p^{3.95\sim 4.16}$ and $2s^{1.68\sim 1.69}2p^{5.01\sim 5.09}$, respectively. On account of the above effects, one can infer that the Cd(1) ion coordination with nitrogen and oxygen atoms is mainly on 4d, 5s, and 5p orbitals. Nitrogen atoms form coordination bonds with Cd(1) ion utilizing 2s and 2p orbitals. The oxygen atoms provide electrons of 2s and 2p to the Cd(1) ion and form coordination bonds. Thus, the Cd(1) ion gained some electrons from four nitrogen atoms of L ligand and two oxygen atoms of pzdc ligands^[30, 31, 32]. Therefore, on the basis of valence-bond theory, the atomic net charge distribution and NBO bond orders of complex **1** (Table 4) exhibits obvious covalent interaction between the coordinated atoms and Cd(1) ion. The differences of NBO bond orders for Cd–O and Cd–N make their bond lengths be different^[31], which is in good agreement with the X-ray crystal structural data of compound **1**.

As can be seen from Fig. 6, the lowest unoccupied molecular orbital (LUMO) mainly consists of L ligand, whereas the highest occupied molecular orbital (HOMO) is mainly composed of pzdc ligand. Thus, the charge transfer from ligand to ligand may be deduced from some contours of molecular orbital of complex **1**.

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Table 1. Selected Bond Lengths (Å) and Bond Angles (°) for 1

Bond	Dist.	Bond	Dist.	Bond	Dist.
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Cd(1)–O(1)	2.514(2)	Cd(1)–O(2B)	2.273(2)	Cd(1)–N(1A)	2.252(3)
Cd(1)–N(2)	2.268(3)	Cd(1)–N(3)	2.371(2)	Cd(1)–N(4)	2.416(3)
Angle	(°)	Angle	(°)	Angle	(°)
N(1A)–Cd(1)–N(2)	97.41(10)	N(1A)–Cd(1)–O(2B)	103.34(10)	N(2)–Cd(1)–O(2B)	71.65(11)
N(1A)–Cd(1)–N(3)	160.98(12)	N(2)–Cd(1)–N(3)	71.57(9)	O(2B)–Cd(1)–N(3)	91.81(11)
N(1A)–Cd(1)–N(4)	95.61(10)	N(2)–Cd(1)–N(4)	161.95(10)	O(2B)–Cd(1)–N(4)	101.84(10)
N(3)–Cd(1)–N(4)	92.39(10)	N(1A)–Cd(1)–O(1)	85.15(9)	N(2)–Cd(1)–O(1)	101.10(8)
O(2B)–Cd(1)–O(1)	167.33(9)	N(3)–Cd(1)–O(1)	81.99(11)	N(4)–Cd(1)–O(1)	67.59(9)

Symmetry codes: A: $-x+5/2, -y+5/2, z$; B: $2-x, -y+5/2, z+1/2$

Table 2. Natural Atomic Charges, Natural Valence Electron Configurations, Wiberg Bond Indexes and NBO Bond Orders (a.u) for 1

Atom	Net charge	Electron configuration	Bond	Wiberg index	bond	NBO bond order
Cd(1)	1.40764	[core]5s(0.29)4d(9.98)5p(0.30)				
O(1)	−0.71875	[core]2s(1.69)2p(5.01)	Cd(1)–O(1)	0.1319		0.1626
O(2)	−0.78169	[core]2s(1.68)2p(5.09)	Cd(1)–O(2)	0.1805		0.2015
N(1)	−0.38097	[core]2s(1.41)2p(3.95)	Cd(1)–N(1)	0.1705		0.2299
N(2)	−0.45175	[core]2s(1.39)2p(4.04)	Cd(1)–N(2)	0.1575		0.2204
N(3)	−0.51005	[core]2s(1.34)2p(4.16)	Cd(1)–N(3)	0.1159		0.1771
N(4)	−0.51750	[core]2s(1.35)2p(4.14)	Cd(1)–N(4)	0.1286		0.1828

Symmetry codes: (A) $-x, -y, z$; (B) $-x+1/2, -y, z-1/2$

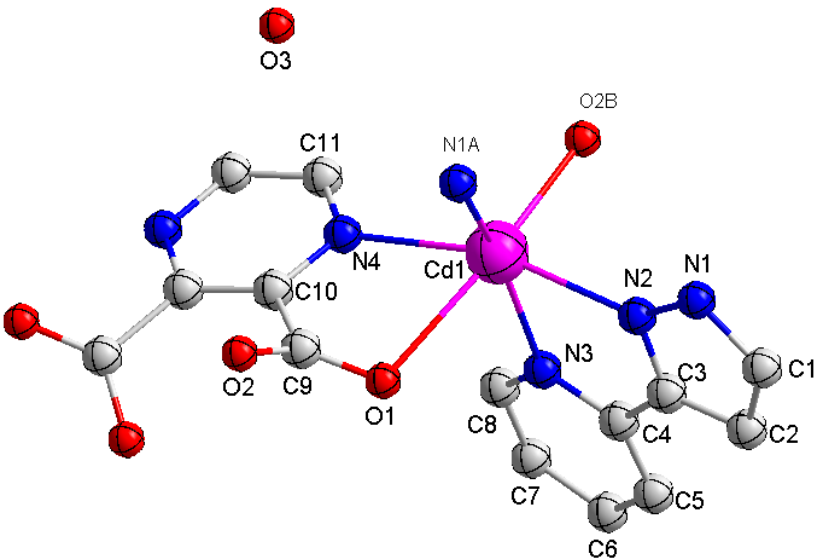


Fig. 1. Coordination environment of the Cd(II) center in 1.

Symmetry codes: (A) $-x+5/2, -y+5/2, z$ (B) $2-x, -y+5/2, z+1/2$

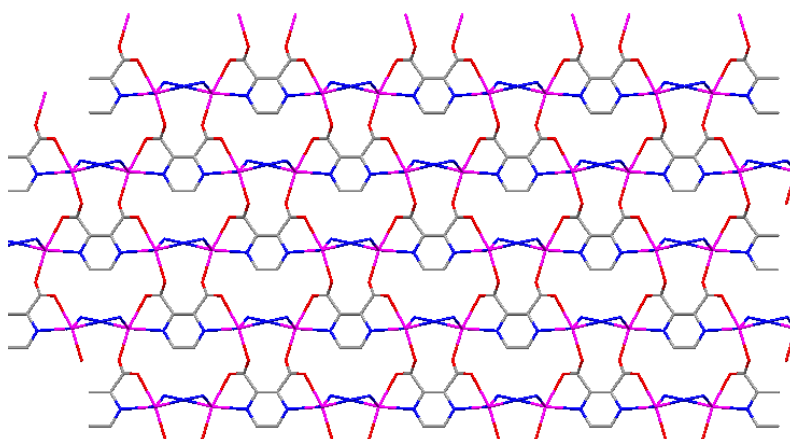


Fig. 2. View of the two-dimensional network structure along the *b* axis
(Carbon atoms of HL ligand were omitted for clarity)

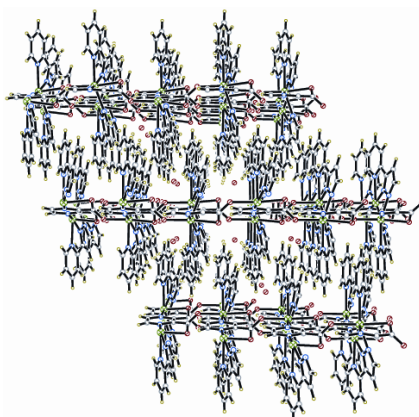


Fig. 3. View of the 3D supramolecular architecture of 1 formed by π - π interactions along the *a* axis
(Carbon atoms of HL ligand were omitted for clarity)

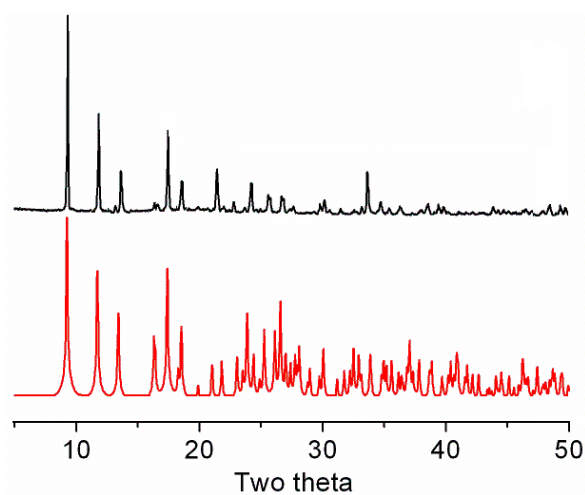


Fig. 4. PXRD analysis of the title complex 1: bottom-simulated, top-experimental

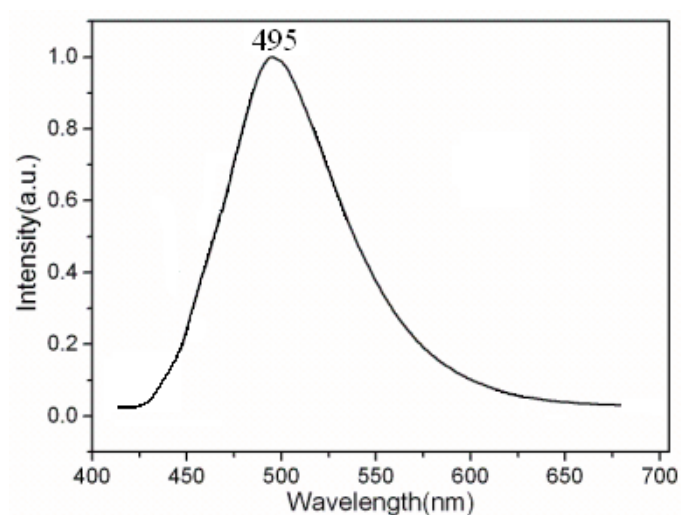


Fig. 5. Solid-state emission spectrum of 1 at room temperature

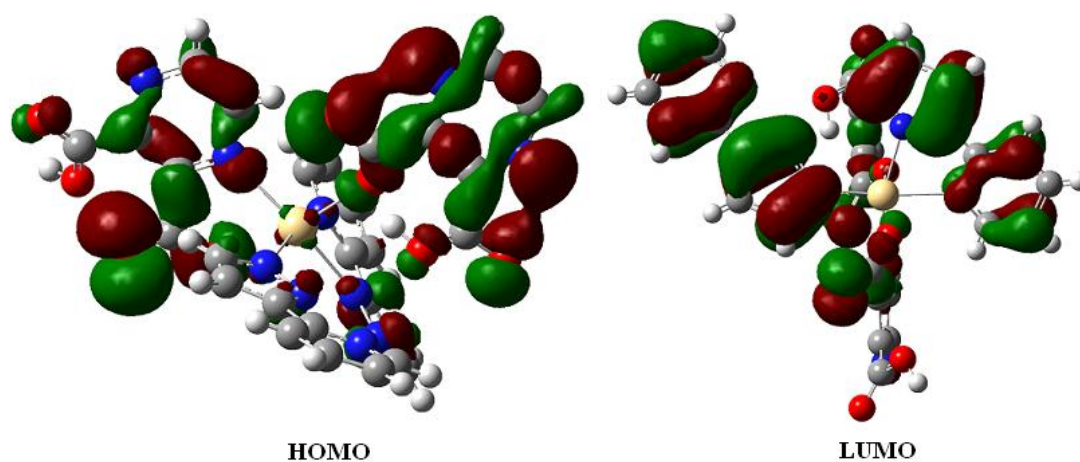


Fig. 6. Frontier molecular orbitals of complex 1

Synthesis, Crystal Structure and Theoretical Calculations of a Three-dimensional Supramolecular Cadmium(II) Coordination Polymer

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A new metal-organic cadmium coordination polymer $[\text{Cd}(\text{pzdc})_{0.5}(\text{L})]_n \cdot n\text{H}_2\text{O}$ has been successfully synthesized under hydrothermal conditions. The structure has been determined by single-crystal X-ray diffraction analysis, elemental analyses, IR and fluorescence spectrum. It shows a two-dimensional network structure and extends into a three-dimensional supramolecular framework through π - π stacking interactions.

